

Energy and structural properties of N -boson clusters attached to three-body Efimov states: Two-body zero-range interactions and the role of the three-body regulator

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The low-energy spectrum of N -boson clusters with pairwise zero-range interactions is believed to be governed by a three-body parameter. We study the ground state of N -boson clusters with infinite two-body s -wave scattering length by performing *ab initio* Monte Carlo simulations. To prevent Thomas collapse, different finite-range three-body regulators are used. The energy and structural properties for the three-body Hamiltonian with two-body zero-range interactions and three-body regulator are in much better agreement with the “ideal zero-range Efimov theory” results than those for Hamiltonian with two-body finite-range interactions. For larger clusters we find that the ground state energy and structural properties of the Hamiltonian with two-body zero-range interactions and finite-range three-body regulators are not universally determined by the three-body parameter, i.e., dependences on the specific form of the three-body regulator are observed. For comparison, we consider Hamiltonian with two-body van der Waals interactions and no three-body regulator. For the interactions considered, the ground state energy of the N -body clusters is—if scaled by the three-body ground state energy—fairly universal, i.e., the dependence on the short-range details of the two-body van der Waals potentials is small. Our results are compared with the literature.

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I. INTRODUCTION

The unitary regime, where the two-body s -wave scattering length is infinitely large, can be reached in ultra cold dilute atomic gases using Feshbach resonance techniques [1]. Two-component Fermi gases were realized experimentally and found to be stable and universal even in the large s -wave scattering length regime [2–4], i.e., the properties of the system were found to be governed, to a very good approximation, by the s -wave scattering length a_s alone and independent of the details of the interaction potential [5–7]. Unitary Bose gases, in contrast, are short-lived [8–10]. Their properties depend on the details of the interaction potential. Typically, this dependence is encapsulated by a three-body parameter [11].

Efimov predicted that three identical bosons interacting through two-body potentials with infinitely large s -wave scattering length a_s and vanishing effective range support an infinite number of three-body bound states [12]. The binding momenta $\kappa_3^{(n)}$ of the trimers (n labels the states) display a geometric scaling, i.e., $\kappa_3^{(n)}/\kappa_3^{(n+1)} \approx 22.6944$ [11, 12]. If the binding momentum of one trimer is known, that of the other trimers is also known. Importantly, the binding momenta themselves cannot be determined solely from a theory that is based on two-body zero-range potentials. Rather, a three-body parameter is needed to regularize the problem (i.e., to set the absolute scale of the three-body spectrum). The three-body regulator can be introduced in many ways. In this work, we consider three different regularization approaches: (i) a Hamiltonian with two-body zero-range potentials and a zero-range three-body potential, (ii) a Hamiltonian with two-body zero-range potentials and a purely repulsive three-body potential,

and (iii) a Hamiltonian with finite-range two-body potentials and no three-body potential.

Much less is known about four- and higher-body systems at unitarity [13–21]. N -body cluster states are believed to be attached to each trimer, i.e., for a trimer with binding momentum $\kappa_3^{(n)}$, two N -body states are believed to exist with binding momenta $C_N^{(1)}\kappa_3^{(n)}$ and $C_N^{(2)}\kappa_3^{(n)}$, where $C_N^{(1)}$ and $C_N^{(2)}$ are dimensionless parameters that do not depend on n . Whether four- and higher-body parameters exist has been under debate in the literature.

The study of N -body states attached to Efimov trimers is challenging for several reasons. To date, no analytical solutions for $N \geq 4$ exist. Numerical treatments have to be capable of describing vastly different length scales. For finite-range two-body interactions, the lowest trimer state is typically not a “pure” Efimov state. Thus, one would ideally like to investigate N -body droplets that are tied to the first- or second-excited trimer states. The corresponding N -body states ($N \geq 4$; see Fig. 1 for an illustration of the four-body spectrum as a function of $1/a_s$) are not bound states but resonance states, which are not stable with respect to break-up into smaller sub-units. Thus, the numerical approach of choice would ideally be capable of treating N -body resonance states whose size is many orders of magnitude larger than the range of the underlying two-body potential.

To bypass these numerical challenges, this work pursues, as have other works before [21, 23], an approach that considers N -body droplets (the thick dashed lines in Fig. 1 show the two four-body states) tied to the energetically lowest-lying trimer state (thick solid line in Fig. 1). To ensure that the trimer ground state has the key characteristics of a true Efimov trimer state, we employ two-body zero-range interactions together with a purely re-

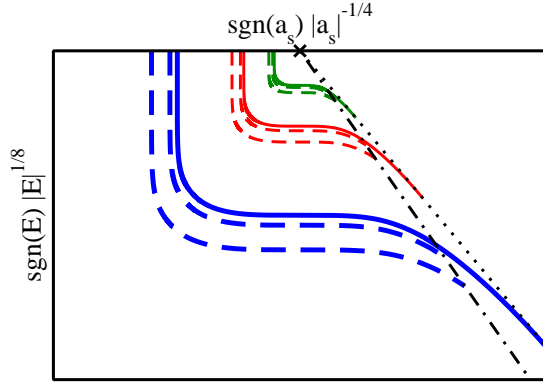


FIG. 1: (Color online) Schematic illustration of the energy spectrum for four identical bosons. The x marks the $(1/a_s, E) = (0, 0)$ point. The dotted line shows the energy of the weakly-bound dimer. The solid lines show different Efimov trimer states, which become unbound on the positive scattering length side at the atom-dimer threshold. The dashed lines show “ground state” and “excited state” tetramers that are attached to each Efimov trimer. These tetramer states hit the dimer-dimer threshold on the positive scattering length side (the energy of the two dimers is shown by the dash-dotted line). It should be noted that the excited tetramer state turns into a virtual state for a certain region of positive scattering lengths [22]; this detail is not reflected in the plot.

TABLE I: Summary of potential models considered in this work. For each model, the two-body potential V_{2b} and the three-body potential V_{3b} are listed. V_{2b} for 2bZR+3bZR, 2bZR+3bHC, and 2bZR+3bRp is the Fermi-Huang pseudopotential [24]; a_s is set to infinity. $V_{ZR}(R)$ for 2bZR+3bZR is treated as a zero-range boundary condition. $V_{HC,R_0}(R)$ is the hardcore repulsive potential; $V_{HC,R_0}(R) = 0$ for $R > R_0$ and $V_{HC,R_0}(R) = \infty$ for $R < R_0$. V_0 and r_0 for 2bG, c_{12} and c_6 for 2bLJ, c_{10} and c_6 for 2b10-6, and c_8 and c_6 for 2b8-6 are chosen such that the s -wave scattering length is infinitely large and the two-body system supports one zero-energy s -wave bound state.

model	V_{2b}	V_{3b}
2bZR+3bZR	$\frac{4\pi\hbar^2}{m} a_s \delta^{(3)}(\mathbf{r}) \frac{\partial}{\partial r} r$	$V_{ZR}(R)$
2bZR+3bHC	$\frac{4\pi\hbar^2}{m} a_s \delta^{(3)}(\mathbf{r}) \frac{\partial}{\partial r} r$	$V_{HC,R_0}(R)$
2bZR+3bRp	$\frac{4\pi\hbar^2}{m} a_s \delta^{(3)}(\mathbf{r}) \frac{\partial}{\partial r} r$	$\frac{C_p}{R^p}$
2bG	$V_0 \exp[-r^2/(2r_0^2)]$	—
2bLJ	$\frac{c_{12}}{r^{12}} - \frac{c_6}{r^6}$	—
2b10-6	$\frac{c_{10}}{r^{10}} - \frac{c_6}{r^6}$	—
2b8-6	$\frac{c_8}{r^8} - \frac{c_6}{r^6}$	—

pulsive three-body potential that serves as a regulator; we refer to this model as 2bZR+3bRp (2b, ZR, 3b, and R stand for two-body, zero-range, three-body, and repulsive, respectively, and p denotes the power of the repulsive three-body potential; see below). The forms of V_{2b} and V_{3b} for the model 2bZR+3bRp are given in Table I and the Hamiltonian H for N particles with mass m and

position vector \mathbf{r}_j reads

$$H = -\sum_{j=1}^N \frac{\hbar^2}{2m} \nabla_j^2 + \sum_{j < k}^N V_{2b}(\mathbf{r}_{jk}) + \sum_{j < k < l}^N V_{3b}(R_{jkl}), \quad (1)$$

where the two-body potential V_{2b} depends on the interparticle distance vector \mathbf{r}_{jk} ($\mathbf{r}_{jk} = \mathbf{r}_j - \mathbf{r}_k$) and the three-body potential V_{3b} depends on the three-body hyperradius R_{jkl} ,

$$R_{jkl} = \sqrt{(\mathbf{r}_{jk}^2 + \mathbf{r}_{jl}^2 + \mathbf{r}_{kl}^2)/3}. \quad (2)$$

Importantly, the N -body Hamiltonian H is well behaved, i.e., the ground state is well defined thanks to the three-body regulator. As we show in Sec. II, the three-body regulator produces three-body states that share many characteristics with the pure three-body Efimov state. Pure three-body Efimov states are obtained if the two-body interactions are of zero range and the hyperradial boundary condition at $R_{123} = 0$ is specified [11]. Since the hyperradial boundary condition or logarithmic derivative can be imposed via a delta-function in the hyperradius, we refer to this model as 2bZR+3bZR.

Our work considers the N -body ground state using a novel Monte Carlo approach [25] that allows for the treatment of two-body zero-range interactions. The Monte Carlo approach can unfortunately not treat three-body zero-range interactions, i.e., it is not capable of treating the Hamiltonian 2bZR+3bZR. A key objective of the present work is then to investigate how the properties of N -body droplets in the ground state, supported by the model Hamiltonian 2bZR+3bRp, change with the number of particles and with the power p of the three-body regulator. An important question is to which degree the N -body properties are determined by the three-body parameter.

For comparison, we also consider Hamiltonian with finite-range two-body Gaussian or van der Waals interactions and no three-body interaction. The ground state manifolds of these models, referred to as 2bG, 2bLJ, 2b10-6, and 2b8-6 (see Table I), lack—as we show—a number of key Efimov characteristics. Two-body Gaussian interactions have been employed extensively in the literature [19, 21, 26–28], sometimes also in combination with a repulsive three-body regulator [23, 29].

Although the structural properties of the ground state trimers for the Hamiltonian with two-body van der Waals interactions differ notably from those for the pure Efimov trimer [30, 31], these systems exhibit universal features [27, 32–39]. Specifically, the trimer ground state binding momentum $\kappa_3^{(1)}$ at unitarity is, to a good approximation, determined by the van der Waals length L_{vdW} [27, 39] and independent of the short-range details. For the two-body Lenard-Jones potential, one finds $\kappa_3^{(1)} \approx 0.230/L_{vdW}$ [40], where $L_{vdW} = (\sqrt{mc_6}/\hbar)^{1/2}/2$. This relationship is nowadays being attributed to van der Waals universality. Moreover, the binding momentum spacing of 23.4 between the ground state and the

first excited state is quite close to the spacing of 22.6944 exhibited by consecutive pure Efimov trimers [40]. It is thus interesting to investigate if van der Waals universality exists for $N > 3$, i.e., to answer the question whether or not the N -body ground state energy depends on the short-range details of the two-body van der Waals potential.

The remainder of this paper is organized as follows. Section II compares the properties of the three-boson system with infinitely large s -wave scattering length interacting through 2bZR+3bZR, 2bZR+3bHC, and 2bZR+3bRp and illustrates the benefits and limitations of these models. Section III reviews several literature results for N -body droplets. Section IV extends the calculations for the 2bZR+3bRp interaction model to clusters with $N \leq 15$. In addition to the energy, various structural properties are discussed in detail. Section V compares the results for the model 2bZR+3bRp with those for systems with two-body finite-range interactions (i.e., for the models 2bG, 2bLJ, 2b10-6, and 2b8-6). Finally, Sec. VI concludes.

II. THREE-BODY SYSTEM AT UNITARITY

To understand the three-body system, it is instructive to rewrite the Hamiltonian H , Eq. (1), for $N = 3$ in hyperspherical coordinates [41]. To this end, we first separate off the center of mass degrees of freedom and restrict ourselves to states with vanishing relative orbital angular momentum. For the 2bZR+3bZR, 2bZR+3bHC, and 2bZR+3bRp models with infinitely large two-body s -wave scattering length a_s , the hyperradial and hyperangular degrees of freedom separate [11, 42]. The lowest eigen value of the hyperangular Schrödinger equation is typically denoted by s_0 , where $s_0 \approx 1.006i$ [11, 12]. This eigen value enters into the hyperradial Schrödinger equation with hyperradial Hamiltonian H_R ,

$$H_R = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial R^2} + \frac{\hbar^2(s_0^2 - 1/4)}{2mR^2} + V_{3b}(R) \quad (3)$$

(for notational simplicity, the three-body hyperradius is denoted by R throughout this section). If $V_{3b}(R)$ is equal to zero, the eigen energies of the Hamiltonian H_R are not well defined. To make the problem well-defined without explicitly introducing a length scale, a boundary condition at $R = 0$, which serves as a regulator and defines a scale, can be specified. This is the model 2bZR+3bZR. The energy spectrum of the 2bZR+3bZR model Hamiltonian displays a perfect geometric series [11]. For an eigen state with binding momentum $\kappa_3^{(n)}$ [the corresponding energy is $(\hbar\kappa_3^{(n)})^2/m$], there exists a tighter and a looser bound state with binding momentum $\kappa_3^{(n-1)} = \exp(\pi/|s_0|)\kappa_3^{(n)}$ and $\kappa_3^{(n+1)} = \exp(-\pi/|s_0|)\kappa_3^{(n)}$, respectively. Here, $\exp(\pi/|s_0|)$ is approximately equal to 22.6944. The three-body spectrum for the 2bZR+3bZR model is not bounded from below;

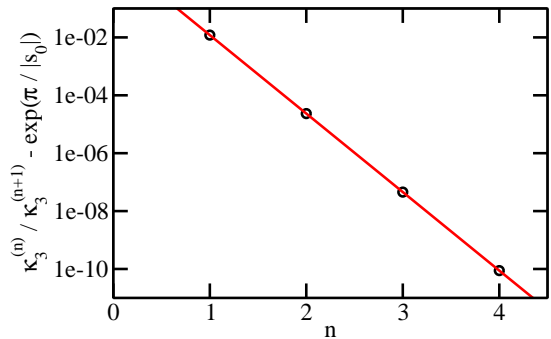


FIG. 2: (Color online) Breaking of the scale invariance for the three-boson system at unitarity with three-body hardcore regulator. The circles show the difference between the binding momentum ratio $\kappa_3^{(n)}/\kappa_3^{(n+1)}$ of the n th and $(n+1)$ th states for the model 2bZR+3bHC and the ratio $\exp(\pi/|s_0|) = 22.6944$ for the model 2bZR+3bZR as a function of n . The solid line shows a fit to the data points. The breaking of the scale invariance becomes weaker with increasing n .

in our notation, this means that n can take non-positive values, i.e., $n = \dots, -2, -1, 0, 1, 2, \dots$. There exists an infinity of three-body bound states and each hyperradial wavefunction $\psi_n(R)$ has infinitely many nodes. The hyperradial wavefunctions of these states collapse if scaled by the binding momentum $\kappa_3^{(n)}$, i.e., $(\kappa_3^{(n)})^{1/2}\psi_n(\kappa_3^{(n)}R)$ is the same for all states.

We now consider finite-range three-body regulators. As a first toy model, we consider a hardcore repulsive three-body potential, i.e., we consider the model 2bZR+3bHC (see Table I). In this case, the hyperangular and hyperradial parts separate as before and the Hamiltonian H_R supports a well defined ground state with energy $E_3^{(1)}$ or binding momentum $\kappa_3^{(1)}$ (in our notation, $n = 1, 2, \dots$). For the n th state with binding momentum $\kappa_3^{(n)}$, the hyperradial wavefunction has $n - 1$ nodes. The circles in Fig. 2 show the difference between the binding momentum ratios for the model 2bZR+3bHC and the model 2bZR+3bZR. The binding momentum ratio for the ground and first excited states of the model 2bZR+3bHC is approximately 22.7064. The deviation from the model 2bZR+3bZR is 0.0120 or 0.053%. As we go to excited states, the deviations decrease exponentially. A log-linear fit of the deviations yields $\kappa_3^{(n)}/\kappa_3^{(n+1)} - \exp(\pi/|s_0|) \approx \exp(1.823 - 6.244n)$ (see the solid line in Fig. 2). The overlap between the wavefunction of the ground state of the model 2bZR+3bHC and the wavefunction of the model 2bZR+3bZR with the same binding momentum is 0.99947, i.e., the inner region where the wavefunction for the model 2bZR+3bHC deviates from the true Efimov wavefunction is insignificant. The three-body hardcore potential breaks the scale-invariance and introduces n -dependent energy spacings.

The discontinuity of the derivative of the wavefunction at $R = R_0$ makes the three-body hardcore regu-

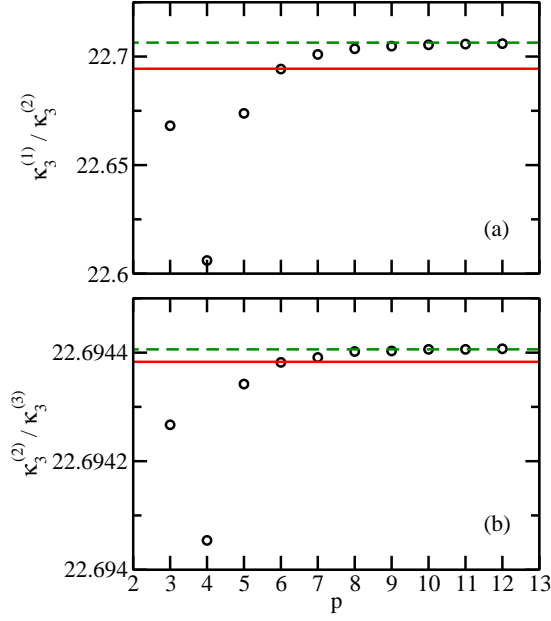


FIG. 3: (Color online) Binding momentum characteristics for the three-boson system with three-body power law regulator at unitarity. The circles show the ratio of the binding momentum of two consecutive states for the model 2bZR+3bRp as a function of p . Panel (a) shows the binding momentum ratio for the ground and the first excited states while panel (b) shows the ratio for the first and the second excited states. The solid and dashed lines show the binding momentum ratio for the models 2bZR+3bZR and 2bZR+3bHC, respectively.

lator challenging to treat numerically, at least by the path integral Monte Carlo (PIMC) technique employed in Sec. IV. Thus, we consider three-body power law potentials, which approach the hardcore potential for $p \rightarrow \infty$. The circles in Fig. 3 show the binding momentum ratios for the model 2bZR+3bRp as a function of p . Figures 3(a) and 3(b) show the binding momentum ratios for the ground and first excited states, and the first and second excited states, respectively. As expected, the binding momentum ratios approach the value for the model 2bZR+3bHC (dashed lines) in the large p limit. For comparison, the solid lines show the binding momentum ratio for the model 2bZR+3bZR. The deviations between the binding momentum ratios for the 2bZR+3bRp and the 2bZR+3bHC models are largest for $p = 4$. Similar to the model 2bZR+3bHC, the binding momentum ratios for the model 2bZR+3bRp approach the value $\exp(\pi/|s_0|)$ exponentially with increasing n .

The spacing of the momenta is not the only way to characterize how universal the system is, i.e., how close a given system is to the true Efimov scenario described by the model 2bZR+3bZR. The structural properties provide additional insights. Indeed, the structures of weakly-bound three-body systems with positive a_s have recently been measured [30, 31]. We first look at the distribution of the angles θ_{jkl} between each pair of position vectors, $\theta_{jkl} = \arccos(\hat{\mathbf{r}}_{jk} \cdot \hat{\mathbf{r}}_{kl})$. The distribution $P_{\text{tot}}(\theta)$

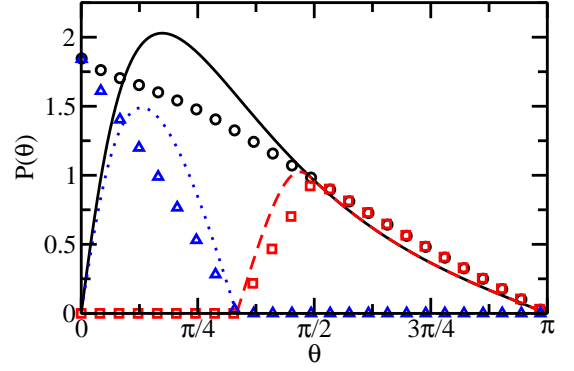


FIG. 4: (Color online) Angular distributions for three identical bosons at unitarity. The circles, triangles and squares show the angular distributions $P_{\text{tot}}(\theta)$, $P_{\text{min}}(\theta)$, and $P_{\text{max}}(\theta)$ for the model 2bZR; these distributions are identical to those for the models 2bZR+3bHC and 2bZR+3bRp. The solid, dotted, and dashed lines show the angular distributions $P_{\text{tot}}(\theta)$, $P_{\text{min}}(\theta)$, and $P_{\text{max}}(\theta)$ for the model 2bG.

considers all three angles of each triangle, while the distribution $P_{\text{min}}(\theta)$ [$P_{\text{max}}(\theta)$] considers only the smallest [largest] of the three angles of each triangle. The normalizations are chosen such that $\int_0^\pi P_{\text{tot}}(\theta)d\theta = 3$ and $\int_0^\pi P_{\text{min}}(\theta)d\theta = \int_0^\pi P_{\text{max}}(\theta)d\theta = 1$. For infinitely large a_s (as considered throughout this section), these angular distributions only depend on the hyperangles and not on the hyperradius. Thus, they are the same for the models 2bZR+3bZR, 2bZR+3bHC, and 2bZR+3bRp. The circles, triangles, and squares in Fig. 4 show $P_{\text{tot}}(\theta)$, $P_{\text{min}}(\theta)$, and $P_{\text{max}}(\theta)$, respectively, for these models. $P_{\text{tot}}(\theta)$ is approximately linear and approaches a finite value for $\theta \rightarrow 0$. We are interested in the angular distributions for two reasons. (i) For the models 2bG, 2bLJ, 2b10-6, and 2b8-6, the hyperangular and hyperradial degrees of freedom do not separate and the difference between their angular distributions and those for the two-body zero-range models provides valuable insights (see Ref. [40]). (ii) For the N -body clusters, the angular distributions, which depend on both the hyperangles and the N -particle hyperradius, can serve to monitor the three-body correlations.

Solid, dotted, and dashed lines in Fig. 4 show the angular distributions $P_{\text{tot}}(\theta)$, $P_{\text{min}}(\theta)$, and $P_{\text{max}}(\theta)$, respectively, of the three-body ground state for the model 2bG. Compared to that for the two-body zero-range models, the angular distribution near $\theta = 0$ for the finite-range model displays distinctly different behavior. For the Gaussian model, the probability of finding an angle of zero is zero and the angular distribution peaks at around 0.17π or 31° . For the zero-range model, the angular distribution peaks at 0 and $P_{\text{tot}}(0)$ is finite. This is because the zero-range boundary condition makes the probability to find two particles at the same position finite. A vanishing interparticle distance corresponds to a triangle in which one of the three angles θ_{jkl} is zero. Since the angular distributions for the models 2bZR+3bZR and

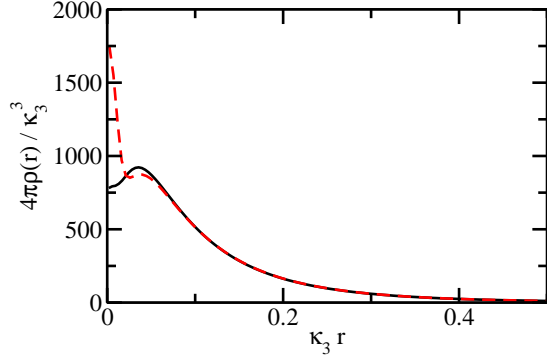


FIG. 5: (Color online) Radial density $\rho(r)$ for three identical bosons at unitarity (r is measured relative to the center of mass of the three-body system). The dashed and solid lines show $\rho(r)$ for the models 2bZR+3bZR and 2bZR+3bRp with $p = 6$, respectively.

2bG show distinctly different features, one might expect that the binding momentum ratios $\kappa^{(1)}/\kappa^{(2)}$ for these two models also differ. The value of $\kappa_3^{(1)}/\kappa_3^{(2)}$ for the model 2bG is 22.983, which differs by only 1.27% from that for the model 2bZR+3bZR. This indicates that it is insufficient to only evaluate the binding momentum ratios to judge how universal the system is. We note that the distribution $P(\theta)$ for the ground state of the $N = 3$ system with two-body Lenard-Jones interactions is quite similar to that for the ground state of the $N = 3$ system with two-body Gaussian interactions [40].

We now consider the radial density $\rho(r)$ (r is measured relative to the center of mass of the three-body system) for the models 2bZR+3bZR and 2bZR+3bRp with $p = 6$. The radial density $\rho(r)$ is normalized such that $4\pi \int_0^\infty \rho(r)r^2 dr = N$ and depends on the hyperradius and the hyperangles. The dashed and solid lines in Fig. 5 show the radial density $\rho(r)$ for the models 2bZR+3bZR and 2bZR+3bRp with $p = 6$, respectively. For the latter, the ground state density is shown. The radial densities are scaled by their respective binding momentum κ_3 . The solid and dashed lines agree well in the large r region and differ notably in the small r region. The deviation in the small r region comes from the fact that the hyperradial density for the model 2bZR+3bZR decays much slower for small R than that for the model 2bZR+3bRp. Note that even though the radial densities for the two models differ by about a factor of two in the small r region, the difference between the integrated contributions is small because the volume element contains an r^2 factor.

III. N -BODY CLUSTERS AT UNITARITY: OVERVIEW OF LITERATURE RESULTS

This section discusses various literature results for the energy of weakly-bound N -body droplets ($N > 3$) at

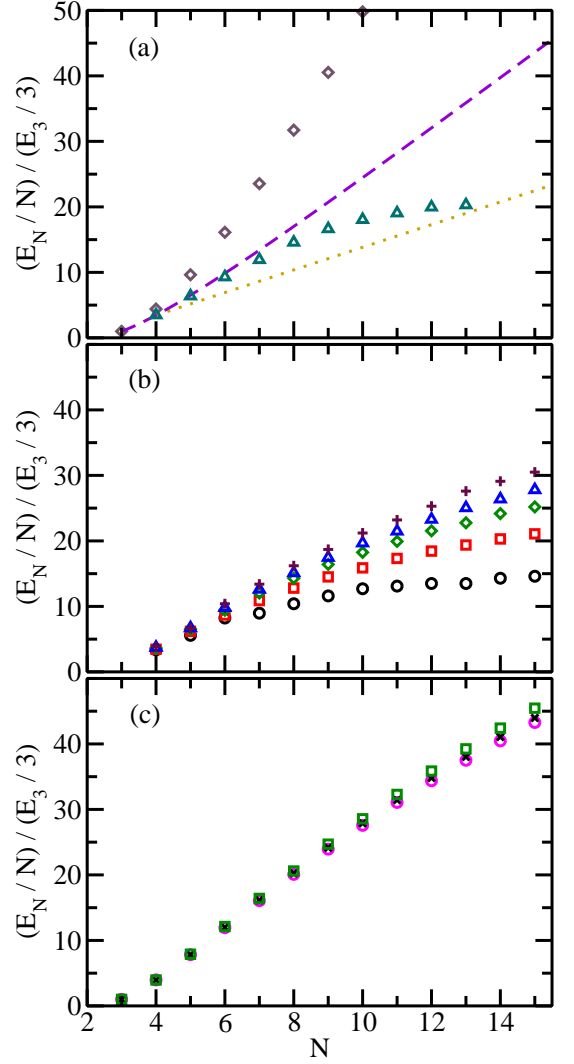


FIG. 6: (Color online) Energy per particle of N -boson clusters at unitarity. (a) Summary of literature results. The dashed and dotted lines show the analytical prediction by Gattobigio and Kievsky [21] and Nicholson [43], respectively. The triangles show the diffusion Monte Carlo (DMC) energies for a Hamiltonian with two-body square well interaction and repulsive three-body hardcore regulator [23]. The diamonds show the energy for the model 2bG [28]. (b) Summary of our PIMC calculations. The circles and pluses are for the model 2bZR+3bRp with $p = 4$ and 8, respectively; the error bars (not shown) are of the order of the symbol sizes. The squares, diamonds, and triangles are for the model 2bZR+3bRp with $p = 5, 6$, and 7, respectively; the error bars (not shown) are smaller than the symbol sizes. (c) Summary of our calculations for two-body van der Waals models. The circles, crosses, and squares show our DMC results for the models 2bLJ, 2b10-6, and 2b8-6, respectively.

unitarity. The diamonds in Fig. 6(a) show the N -boson energy per particle E_N/N for the model 2bG as a function of N [21, 26, 28]. The energy per particle increases approximately linearly with N for $N > 6$ (for smaller N , some deviations from the linear behavior exist). Based

on the fact that the energy per particle, and correspondingly the binding momentum, scale linearly with N for the model 2bG, Gattobigio *et al.* [21] proposed an analytical form for the N -boson system with two-body zero-range interactions and fixed three-body parameter,

$$\frac{\kappa_N}{\kappa_3} = 1 + \left(\frac{\kappa_4}{\kappa_3} - 1 \right) (N - 3) \quad (4)$$

[see the dashed line in Fig. 6(a)]. The ratio κ_4/κ_3 is not taken from the ground state calculations for the Gaussian two-body interaction model, for which $\kappa_4/\kappa_3 = \sqrt{5.86}$, but from Deltuva's calculations for highly excited four-body resonance states. Deltuva finds the universal ratio $\kappa_4/\kappa_3 = \sqrt{4.61}$ [17]. Gattobigio *et al.*'s expression, converted to the energy, exhibits a leading order N^2 and sub-leading order N dependence.

It should be noted that the ground state energy of the Hamiltonian with pairwise Gaussian interactions scales differently with N for $N \gtrsim 10$ than that of Hamiltonian with pairwise interactions with short-range repulsion. For interactions with repulsive core, it is well established that the energy per particle increases weaker than linear for $N \gtrsim 10$ (see, e.g., the literature on helium and tritium droplets [44, 45]). Gattobigio *et al.* [26] noted that Eq. (4) applies not only to systems with zero-range interactions but also to systems with finite-range interactions in the regime where E/N is approximately proportional to N (e.g., to helium droplets with $N \lesssim 10$). In this case, the ratio κ_4/κ_3 for the finite-range potential is taken as input and the binding momentum for $N > 4$ is predicted. We return to this discussion in Sec. V.

Independent evidence for the leading-order N dependence of the energy per particle for the Hamiltonian with two-body zero-range interactions comes from lattice calculations for even N [43]. Assuming that the distribution of the two-body correlator is exactly log normal, Nicholson deduced an analytical expression for the energy per particle, $E_N/N = (N/2 - 1)E_4/4$ [see the dotted line in Fig. 6(a)] [43]. To plot this expression, we used Deltuva's value of $E_4/E_3 = 4.61$. It should be noted that the coefficients predicted by Gattobigio *et al.* and Nicholson for the leading order N dependence differ by about a factor of 2.

A somewhat different N -dependence of the energy per particle was observed in the numerical calculations by von Stecher [see triangles in Fig. 6(a)] [23]. In fact, the idea to use a three-body regulator, as in our model 2bZR+3bRp, to make the ground state trimer large and Efimov-like was introduced in Ref. [23]. Von Stecher employed a model Hamiltonian with two-body square well potential with infinitely large two-body s -wave scattering length and three-body hardcore potential. For $N \lesssim 10$, the energy per particle increases approximately linearly with increasing N . For larger N , the triangles in Fig. 6(a) flatten. Reference [46] interpreted this as a turnover to a N^0 dependence of the energy per particle. Such a behavior suggests a saturation of the density for large N . This saturation would be a consequence of the balance

of the two-body attractive and three-body repulsive interactions.

The discussion above shows that the dependence of the energies tied to Efimov trimers is not well understood. Specifically, neither the functional form of the energy per particle nor the coefficients are agreed upon. In the following sections, we attempt to understand where the discrepancies of the literature results come from.

IV. N -BODY RESULTS AT UNITARITY FOR THE MODEL 2bZR+3bRp

To calculate the N -boson energy for the Hamiltonian with interaction model 2bZR+3bRp, we apply the PIMC technique [25, 47]. The PIMC technique is an, in principle, exact finite-temperature method; the errors, which originate from the discretization of the imaginary time and the stochastic evaluation of integrals, can be reduced systematically. To obtain the ground state energy of the N -boson Hamiltonian, the PIMC approach has to be extended to the zero-temperature limit. Typically, this is achieved by the path integral ground state approach [47, 48]. Here, we pursue an alternative strategy. Namely, we work in the finite temperature regime where the thermal contribution to the energy is known and where the structural properties of interest are not affected by the temperature. This approach was introduced and benchmarked in Ref. [28]. The basic idea is to place the droplet in a weak external harmonic confinement, whose angular frequency ω is chosen such that the center of mass energy spectrum becomes discretized and the relative motion is unaffected by the trap. This requirement corresponds to $|E_N| \gg \hbar\omega$. Since the density of states of the harmonically trapped center of mass pseudoparticle is known analytically, the ground state energy E_N of the N -boson droplet in free space can be extracted from the finite-temperature energy [25, 28].

The circles, squares, diamonds, triangles, and pluses in Fig. 6(b) show the energy per particle for the model 2bZR+3bRp with $p = 4, 5, 6, 7$, and 8, respectively, as a function of N (see also Table II and the Supplemental Material [54]). For each p , the energy per particle is scaled by the respective trimer energy per particle. For a fixed p , the energy per particle increases monotonically and smoothly as a function of N , i.e., even-odd effects, which have been observed in trapped and homogeneous two-component Fermi gases [49–51], are—if existent—smaller than our statistical error bars. For fixed N , the scaled energy per particle increases with increasing p ($p \geq 4$); this increase becomes smaller with increasing p . Similarly to von Stecher's energy per particle [23] [triangles in Fig. 6(a)], the scaled energy per particle increases roughly linearly for smallish N and then flattens out for larger N . This effect is most pronounced for $p = 4$ and 5, where the flattening sets in around $N = 8 - 10$, and least pronounced for $p = 8$. The reason for the flattening is that the clusters develop, for sufficiently large N , more

TABLE II: PIMC energies for the model 2bZR+3bRp for $N = 4 - 15$. Columns 2-4 show the scaled energy $E_N/N/(E_3/3)$ for $p = 5, 6$, and 7 , respectively. The error bars (not explicitly reported) are around 3%.

N	2bZR+3bR5	2bZR+3bR6	2bZR+3bR7
4	3.46	3.64	3.73
5	6.19	6.53	6.70
6	8.69	9.42	9.81
7	10.9	12.0	12.6
8	12.8	14.3	15.1
9	14.5	16.4	17.5
10	15.9	18.3	19.7
11	17.3	20.0	21.5
12	18.4	21.5	23.3
13	19.4	22.8	25.0
14	20.3	24.2	26.4
15	21.1	25.2	27.8

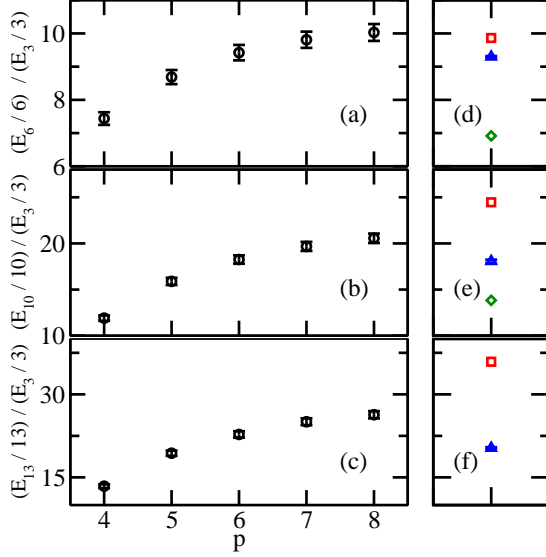


FIG. 7: (Color online) Comparison of our PIMC energies (left) and literature results (right) for selected N . Panels (a), (b), and (c) show our PIMC energy per particle for N -boson clusters interacting through the model 2bZR+3bRp as a function of p for $N = 6, 10$, and 13 , respectively. For comparison, panels (d), (e), and (f) show the energy per particle from the literature for the same N . The triangles, diamonds, and squares are from von Stecher [23], Nicholson [43], and Gattobigio *et al.* [21]. Since the work by Nicholson is restricted to even N , comparison for $N = 13$ cannot be made.

than one pair distance scale (see below for more details).

The circles in Fig. 7 replot the PIMC energy per particle for selected N . As the power p increases, the scaled energy approaches a constant. Based on our discussion in Sec. II, the $p \rightarrow \infty$ energy should coincide with the energy for the model 2bZR+3bHC. It is thus instructive to compare our scaled energies, extrapolated by eye to the $p \rightarrow \infty$ limit, with those obtained by von Stecher [23], who employed a two-body square well potential and a three-body hardcore regulator [see triangles in Figs. 7(d)-

7(f)]. We find that our $p \rightarrow \infty$ energy per particle lies above von Stecher’s energy per particle by something like 10 – 20%, 20 – 30%, and 30 – 50% for $N = 6, 10$, and 13 , respectively. Since the three-body sectors are treated on consistent footing (3bRp \rightarrow 3bHC as $p \rightarrow \infty$), we speculate that the difference arises from the different two-body interactions. However, we did not perform calculations to confirm this and can thus not rule out other reasons. As can be seen from Fig. 7, Nicholson’s energy prediction lies notably below our large p energies while Gattobigio *et al.*’s prediction lies above our large p energies for $N \gtrsim 8$.

If the N -body energies were determined solely by a three-body parameter κ_3 , the model 2bZR+3bRp for different p would yield the same scaled energies, i.e., the symbols in Fig. 6(b) would collapse to a single curve. The fact that they do not collapse indicates that the three-body parameter is not sufficient to predict the energy of the N -boson clusters, at least not for the models considered. To gain more insight into this, it is instructive to analyze the length scales of the model 2bZR+3bRp. Four length scales can be identified (see rows 3–6 of Table III). (i) The characteristic length scale L_p of the three-body repulsive potential. (ii) The length scale \bar{L}_3 defined by the three-body binding energy. (iii) The length scale \bar{L}_N defined by the energy of the cluster. And, (iv) the length scale \bar{l}_N associated with the energy per particle of the cluster. Inspection of the definitions given in Table III shows that \bar{L}_N and \bar{l}_N are not independent.

For $p = 4-8$, we find $\bar{L}_3/L_p \approx 29.3, 28.8, 27.6, 26.6$, and 25.9 , i.e., the trimer is significantly larger than the scale of the underlying repulsive three-body potential. This ensures, as discussed in Sec. II, that the trimer ground state described by the model 2bZR+3bRp with $p \geq 4$ exhibits the key characteristics of an Efimov state. It is instructive to alternatively think about the trimer size in terms of the average interparticle spacing \bar{r} . For trimers with $p = 4-8$, we find $\bar{r}/L_p \approx 18.7, 18.5, 17.7, 17.1$, and 16.6 .

For $p = 6$, we find that \bar{L}_N/L_p changes from 11.2 for $N = 4$ to 8.37 for $N = 5$ to 2.46 for $N = 15$. This suggests that the N -boson droplet “sees” increasingly more of the three-body regulator as N increases, i.e., that the dependence of E_N/N on p increases with increasing N . The length scale \bar{l}_N , in contrast, suggests a larger separation of scales; for $N = 13$, e.g., we have $\bar{l}_N/L_p = 7.69$ for $p = 4$ and $\bar{l}_N/L_p = 6.85$ for $p = 8$. In fact, if E_N/N scales as N , then \bar{L}_N and \bar{l}_N scale as $1/N$ and $1/\sqrt{N}$, respectively. If E_N/N scales as N^0 , then \bar{L}_N and \bar{l}_N scale as $1/\sqrt{N}$ and N^0 , respectively. This implies that—unless the energy scales linearly (or even weaker) with N for large N —the properties of the N -boson droplets are expected to be notably affected by the choice of the three-body regulator.

Alternatively, one can consider the average interparticle distance \bar{r} and the average sub-three-body hyperradius \bar{R} . The squares in Fig. 8(a) show the average interparticle spacing \bar{r} , i.e., the expectation value of the pair distance, as a function of N in units of $1/\kappa_3$ (left axis)

TABLE III: Summary of the definitions of length scales. The van der Waals length L_{vdW} is defined in Ref. [1]. L_p for $p = 6$ agrees with L_{vdW} if m is replaced by the reduced two-body mass $m/2$.

length scale	definition	description
L_g	r_0	characteristic length scale of the two-body Gaussian potential
L_{vdW}	$(\sqrt{m}c_6/\hbar)^{1/2}/2$	characteristic length scale of the two-body van der Waals potential
L_p	$[1/(p-2)\sqrt{2mC_p/\hbar}]^{2/(p-2)}$	characteristic length scale of the three-body repulsive potential
\bar{L}_3	$1/\kappa_3 = \hbar/\sqrt{m E_3 }$	length scale set by the three-body binding energy
\bar{L}_N	$1/\kappa_N = \hbar/\sqrt{m E_N }$	length scale set by the N -body binding energy
\bar{l}_N	$\hbar/\sqrt{m E_N /N} = \sqrt{N}\bar{L}_N$	length scale set by the N -body binding energy per particle
\bar{r}		average interparticle spacing
\bar{R}		average sub-three-body hyperradius

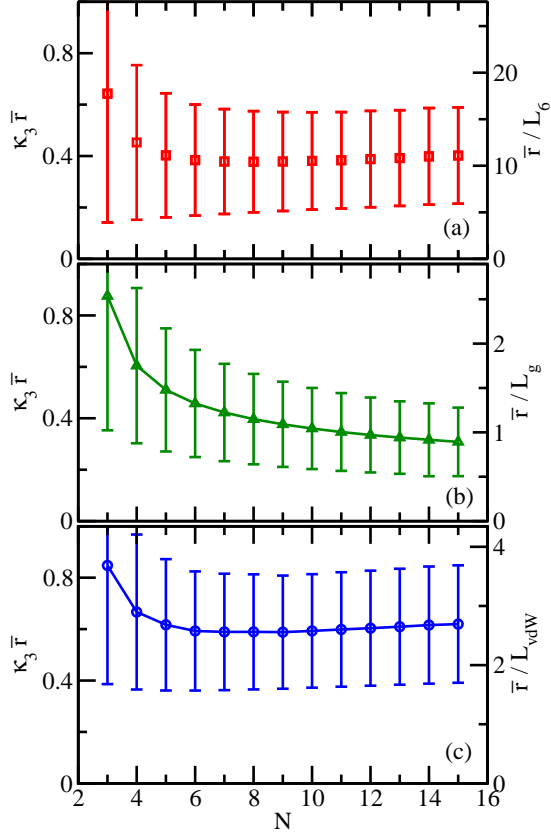


FIG. 8: (Color online) Expectation value \bar{r} of the pair distance as a function of N for N -boson systems interacting through various models. (a) The squares are for the model 2bZR+3bRp with $p = 6$. (b) The triangles are for the model 2bG. (c) The circles are for the model 2bLJ. The error bars show the variance of the pair distance. The pair distances are plotted using two different units: (i) the inverse three-body binding momentum (left axis) and (ii) the characteristic length scale of the model Hamiltonian (right axis).

and in units of L_6 (right axis) for the model 2bZR+3bRp with $p = 6$. The error bars indicate the variance Δr of the pair distance, $\Delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2}$, where $\langle \rangle$ indicates the quantum mechanical expectation value [55]. As the number of particles N increases, both the mean and variance of the pair distance are nearly constant. The mean

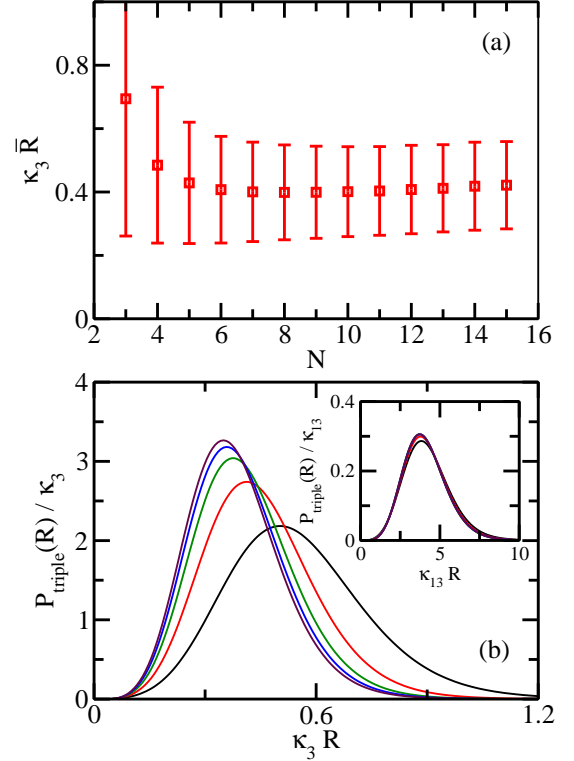


FIG. 9: (Color online) (a) Expectation value \bar{R} of the sub-three-body hyperradius (triple size) as a function of N for N -boson systems interacting through the model 2bZR+3bRp6. The error bars show the variance of the triple size. (b) Triple distribution function $P_{\text{triple}}(R)$ for the $N = 13$ cluster scaled using the three-body binding momentum κ_3 . The solid lines from top to bottom at $\kappa_3 R = 0.6$ are for the model 2bZR+3bRp with $p = 4, 5, 6, 7$, and 8. The inset replots the triple distribution functions using the binding momentum κ_{13} of the $N = 13$ droplet. In these units, the triple distribution functions for different p collapse.

and variance of the pair distance are about one order of magnitude larger than the internal length scale L_p . The relatively large variance of the Hamiltonian with model interaction 2bZR+3bRp implies that the clusters are diffuse and liquid-like. The squares in Fig. 9(a) show the average sub-three-body hyperradius \bar{R} , i.e., the expectation

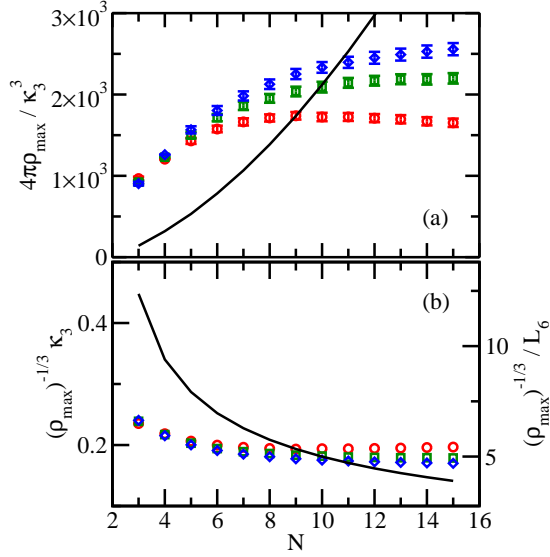


FIG. 10: (Color online) (a) Maximum density ρ_{\max} as a function of N for N -boson systems interacting through various models. The circles, squares, and diamonds are for the model 2bZR+3bRp with $p = 5$ (lowest data set), 6, and 7 (highest data set), respectively. For comparison, the line is for the model 2bG. (b) Same data as in (a) but replotted as the minimum average interparticle distance $(\rho_{\max})^{-1/3}$. The right axis shows the data for the model 2bZR+3bR6 in units of L_6 .

value of the triple size, as a function of N for the model 2bZR+3bRp with $p = 6$. The error bars indicate the variance. The mean and variance of the sub-three-body hyperradius behave similar to the mean and variance of the pair distance.

The average pair distance and sub-three-body hyperradius are obtained by averaging over all possible pairs and triples regardless of whether or not the particles are close to each other. To get more “local” information, we calculate the maximum density and subsequently the closest pair distance. The circles, squares, and diamonds in Fig. 10(a) show the maximum ρ_{\max} of the radial density for the model 2bZR+3bRp with $p = 5, 6$, and 7, respectively, as a function of N . We find that unlike for $N = 3$ (see Fig. 5), the radial density peaks at $r = 0$ for $N \geq 4$. For all p , the maximum of the radial density is roughly a constant for the largest N considered. This constant depends—as the energy per particle—on the three-body regulator. The circles, squares, and diamonds in Fig. 10(b) show the smallest average pair distance for the model 2bZR+3bRp with $p = 5, 6$, and 7, respectively, as a function of N . The smallest average pair distance decreases with increasing N and approximately saturates for the largest N considered. The smallest average pair distance is only about five times larger than the characteristic length scale L_p of the three-body regulator.

The above length scale discussion can be expanded by considering distribution functions. The scaled pair distribution function $4\pi r^2 P_{\text{pair}}(r)$, normalized according to

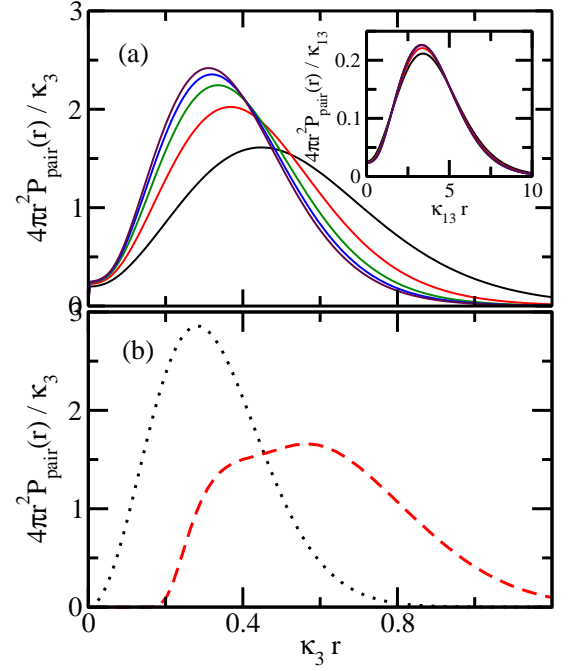


FIG. 11: (Color online) Scaled pair distribution function $4\pi r^2 P_{\text{pair}}(r)$ for $N = 13$ bosons interacting through various models. (a) The solid lines from top to bottom at $\kappa_3 r = 0.8$ are for the model 2bZR+3bRp with $p = 4-8$, scaled using the three-body binding momentum κ_3 . The inset replots the pair distribution functions scaled using the binding momentum κ_{13} of the $N = 13$ droplet. In these units, the pair distribution functions for different p collapse. (b) The dashed and dotted lines show the scaled distribution functions for the models 2bLJ and 2bG, respectively, using the three-body binding momentum κ_3 .

$4\pi \int_0^\infty r^2 P_{\text{pair}}(r) dr = 1$, tells one the probability to find two particles at a distance r from each other. The lines from top to bottom at $\kappa_3 r = 0.8$ in Fig. 11(a) show the scaled pair distribution function $4\pi r^2 P_{\text{pair}}(r)$ for $N = 13$ interacting through 2bZR+3bRp with $p = 4-8$. The amplitude at $r = 0$ is finite and roughly independent of p . This makes sense as it is a signature of the two-body zero-range interactions, which enforce a finite amplitude at $r = 0$.

The triple distribution function $P_{\text{triple}}(R)$, normalized according to $\int_0^\infty P_{\text{triple}}(R) dR = 1$, tells one the probability to find three particles with sub-three-body hyperradius R . The solid lines from top to bottom at $\kappa_3 R = 0.6$ in Fig. 9(b) show the triple distribution function $P_{\text{triple}}(R)$ for $N = 13$ interacting through 2bZR+3bRp with $p = 4-8$. The triple distribution functions are broad and structureless, indicating that the clusters are diffuse and liquid-like and that no small three-body sub-systems are formed.

Figures 9(b) and 11(a) show that the distribution functions $P_{\text{pair}}(r)$ and $P_{\text{triple}}(R)$ do not collapse if scaled by the three-body binding momentum κ_3 . The distribution functions for $p = 4$ are notably broader than those for

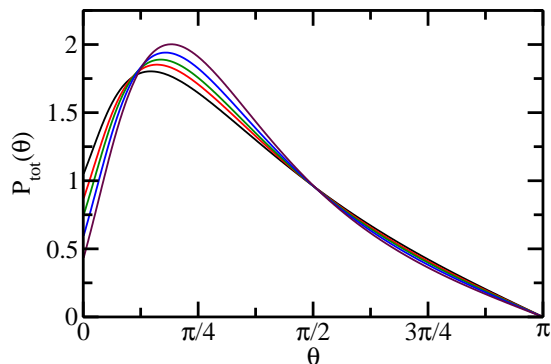


FIG. 12: (Color online) Angular distribution $P_{\text{tot}}(\theta)$ for N -boson clusters interacting through the model 2bZR+3bRp with $p = 6$. The lines from top to bottom at $\theta = 0$ are for $N = 5, 6, 7, 9$, and 13 .

$p > 4$. Figures 9(a) and 11(a) suggest that the distribution functions converge in the large p limit (i.e., in the three-body hardcore regulator limit). Similar behavior is observed for other N . As shown in the insets of Figs. 9(b) and 11(a), the distribution functions collapse to a very good approximation to a single curve if scaled by the binding momentum κ_N of the N -body droplet. This can be understood as a new type of universality, which is weaker than the “Efimov universality”: The binding momentum κ_N allows one to collapse the distribution functions for the models 2bZR+3bRp for sufficiently large p but κ_N is not determined by κ_3 (the latter would constitute “Efimov universality”). The dominance of κ_N arises because the vast majority of the wave function amplitude is located in the classically forbidden region [52] (for pure zero-range interactions, the classically allowed region is reduced to a single point).

At the three-body level, the angular distribution functions for the models 2bZR+3bRp and 2bZR+3bZR coincide since the hyperradial and hyperangular degrees of freedom separate. This is not the case for $N > 3$, since the three-body regulator depends on the N -body hyper-radius and a subset of the $3N - 4$ hyperangles. For fixed N , we find that the dependence of the angular distribution functions $P_{\text{tot}}(\theta)$ on the power p of the three-body regulator is small [much smaller than the dependence of $P_{\text{pair}}(r)$ and $P_{\text{triple}}(R)$ on p]. Figure 12 shows the angular distribution function $P_{\text{tot}}(\theta)$ for N -boson clusters interacting through 2bZR+3bR6 for various N . The lines from top to bottom at $\theta = 0$ are for $N = 5, 6, 7, 9$, and 13 . As the number of particles increases, the probability of finding triangles with small angles decreases but remains finite. Intuitively, this is because $P_{\text{tot}}(\theta)$ accounts for all the trimer configurations and not just the “closest trimers”.

Combining the information displayed in Figs. 6–12, the key characteristics of the ground state of N -boson droplets interacting through the model 2bZR+3bRp with $p \geq 4$ can be summarized as follows: (i) The dependence of the energy and the structural properties on the

three-body regulator decreases with increasing p ; (ii) the dependence of the energy and the structural properties on the three-body regulator cannot be explained by simple length scale arguments (the separation of scales is largest for the $p = 4$ regulator and smallest for the $p = 8$ regulator); (iii) the pair and triple distribution functions collapse to a very good approximation to a single curve if scaled by the binding momentum of the N -body system, suggesting that $1/\kappa_N$ and not $1/\kappa_3$ is the governing length scale for $N > 3$.

V. RESULTS FOR OTHER INTERACTION MODELS

We now compare the findings for N -boson systems interacting through the model 2bZR+3bRp with $p = 4 - 8$ (see the previous section) with those for N -boson systems interacting through the models 2bG, 2bLJ, 2b10-6 and 2b8-6.

We start our discussion with the model 2bG, for which the energy per particle scales, to a very good approximation, linearly with N for $N \gtrsim 6$ [see diamonds in Fig. 6(a)]. The model 2bG has no repulsive core and is characterized by a single length scale, the width r_0 . Using a simple variational Gaussian product wave function in the single-particle coordinates, one can readily show that the ground state energy scales as N^2 and that the peak density increases quadratically with N . Indeed, our calculations shown in Figs. 8(b) and 10 for up to $N = 15$ clearly support that the droplet shrinks with increasing N . As can be seen in Fig. 8(b), the average interparticle distance quickly decreases to a value smaller than r_0 . We conclude that the N^2 scaling of the energy for the model 2bG predominantly reflects the absence of a repulsive core in the potential energy and less so Efimov characteristics.

Next, we discuss the properties of the Hamiltonian interacting through the van der Waals models 2bLJ, 2b10-6, and 2b8-6. Our calculations at unitarity are performed using the same atomic mass and the same c_6 coefficient for the three models while the short-range coefficients are tuned such that the dimer supports a single s -wave bound state with zero energy. For the three-body system, we find $\kappa_3 L_{\text{vdW}} = 0.230$ for the model 2bLJ, $\kappa_3 L_{\text{vdW}} = 0.233$ for the model 2b10-6, and $\kappa_3 L_{\text{vdW}} = 0.245$ for the model 2b8-6, i.e., the three-body binding momentum depends weakly on the short-range scale of the two-body potential. The N -body energies per particle, in units of the three-body energy per particle, are summarized in Table IV. These energies are obtained by the DMC approach [53]. Dividing the N -body energies by the corresponding three-body energy, the energy per particle curves for the three van der Waals interaction models nearly collapse [see Fig. 6(c)]. This can be interpreted as van der Waals universality in the N -body sector. Due to the repulsive core, the energy per particle flattens around $N = 10$, indicating that the system starts

TABLE IV: DMC energies for the Hamiltonian with two-body van der Waals interactions for $N = 4 - 15$. Columns 2-4 show the scaled energy $E_N/N/(E_3/3)$ for the models 2bLJ, 2b10-6, and 2b8-6, respectively. The error bars (not explicitly reported) are around 1%.

N	2bLJ	2b10-6	2b8-6
4	3.978	3.953	3.960
5	7.827	7.841	7.887
6	11.95	11.99	12.12
7	16.07	16.15	16.40
8	20.09	20.24	20.59
9	23.94	24.15	24.69
10	27.57	27.89	28.57
11	31.07	31.44	32.29
12	34.37	34.81	35.86
13	37.50	38.02	39.25
14	40.46	41.06	42.41
15	43.27	43.97	45.46

to grow outward, i.e., starts to form a “second layer” (of course, the system is liquid-like and individual layers cannot be identified). Consistent with this, Fig. 8(c) shows that the average interparticle distance first decreases with increasing N and then slowly increases for $N \gtrsim 8$.

The dashed line in Fig. 11(b) shows the pair distribution function of the $N = 13$ system interacting through the model 2bLJ. The amplitude in the small r region is suppressed compared to the other interaction models considered due to the repulsive two-body core. Scaling $r^2 P_{\text{pair}}(r)$ using κ_{13} (not shown) does not bring the pair distribution function for the model 2bLJ in agreement with the scaled pair distribution functions shown in the inset of Fig. 11(a) for the model 2bZR+3bRp with $p = 4 - 8$. This reflects the fact that a notably smaller fraction of the wave function amplitude resides in the classically forbidden region for the model 2bLJ than for the model 2bZR+3bRp with $p = 4 - 8$.

As already mentioned in Sec. III, Eq. (4) applies, according to Ref. [26], not only to systems with zero-range interactions but also to systems with finite-range two-body interactions. To assess the applicability of Eq. (4), we denote the left hand side of Eq. (4) by $\kappa_N^{\text{appr}}/\kappa_3$ and plot the normalized difference between $\kappa_N^{\text{appr}}/\kappa_3$ and the exact κ_N/κ_3 , as determined by our calculations. Circles and triangles in Fig. 13 shows the quantity $(\kappa_N^{\text{appr}} - \kappa_N)/\kappa_N$ for the models 2bG and 2bLJ, respectively. For $N = 3$ and $N = 4$, the normalized difference is zero by construction. For $N > 4$, the normalized difference is negative for the model 2bG and positive for the model 2bLJ. The deviations from the functional form proposed by Gattobigio *et al.* increase roughly linearly with N for the model 2bLJ, reaching 13% for $N = 15$, and non-linearly for the model 2bG, reaching -20% for $N = 15$. Thus if high accuracy predictions are sought, then Eq. (4) should be used with caution.

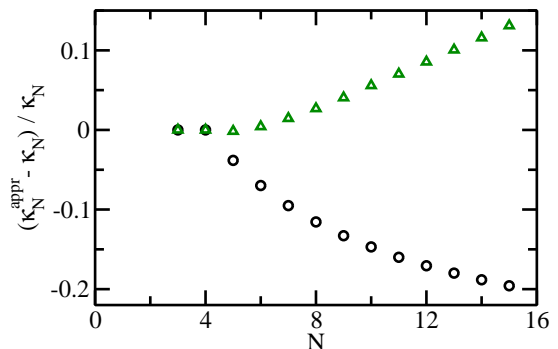


FIG. 13: (Color online) Assessing the applicability of Eq. (4) for N -boson systems with two-body finite-range interactions at unitarity. Circles and triangles show the normalized difference $(\kappa_N^{\text{appr}} - \kappa_N)/\kappa_N$ for the models 2bG and 2bLJ, respectively, as a function of the number of particles N .

VI. CONCLUSIONS

This paper studied weakly-bound Bose droplets at unitarity. These systems are obtained by adding one atom at a time to an Efimov trimer or a weakly-bound trimer with Efimov characteristics. We carefully analyzed the three-body system and then studied larger systems.

The three-body ground state of the Hamiltonian with two-body zero-range interactions and repulsive three-body potential (model 2bZR+3bRp) is a nearly ideal Efimov state. The premise was (see also Ref. [23]) that this would allow us to determine the universal properties of droplets tied to a three-body Efimov state by studying N -body ground states. Somewhat surprisingly, we found dependences of the ground state cluster properties on the three-body regulator, suggesting that the ground states become less universal with increasing N . This is a somewhat disappointing finding as the treatment of N -body excited and resonance states, which are expected to exhibit universal characteristics, is a computationally much more demanding task. Yet, our study revealed a different type of universality for these model Hamiltonian. We found that if the lengths are scaled by the N -body binding momentum, then the dependence on the three-body regulator diminishes notably. This suggests that the ground states of these systems are halo states [52], i.e., states whose amplitude is predominantly located in the classically forbidden region. The N -body binding momentum itself is, however, not—as it would be in the case of N -body Efimov universality—determined by the three-body binding momentum, especially not as N increases.

Hamiltonian with two-body van der Waals interaction at unitarity were also investigated. It was found that the energy per particle, if scaled by the three-body energy, collapses to a very good approximation to a single curve, suggesting that the short-range details of the van der Waals interaction impact the three- and higher-body sectors in a similar manner (i.e., the short-range

details are to a very good approximation “taken out” by scaling by the three-body energy). The calculations presented were for Lenard-Jones and modified Lenard-Jones potentials; the latter potentials have a $-c_6/r^6$ tail but a softer repulsive core at small distances than typical van der Waals interactions. We also performed calculations for (i) the true helium-helium potential scaled by an overall factor such that the s -wave scattering length is infinitely large and (ii) the true helium-helium potential with modified short-range potential such that the s -wave scattering length is infinitely large (these models were labeled He-He(scale) and He-He(arctan) in Ref. [40]). The energy per particle curves for these systems, which have a more complicated long-range tail, also collapse, to a very good approximation, to the same curves as those for 2bLJ, 2b10-6, and 2b8-6 if scaled by the three-body energy. The structural properties, specifically the pair and triple distribution functions, for the van der Waals systems do not collapse to the same curves as those for the 2bZR+3bRp model with $p = 4 - 8$ if scaled using the N -body binding momentum κ_N , suggesting that a good portion of the wave function amplitude of the van der Waals systems is located in the classically allowed

region.

In the future, it would be interesting to extend the calculations presented here to excited and resonance states. We expect that the N -body properties become universal if sufficiently high excitations are being considered. In the four-body sector, e.g., Deltuva [17] extracted the universal numbers for κ_4/κ_3 by going to high-lying resonance states (in this case, “high-lying” means third or higher resonance states). Extending calculations such as those conducted by Deltuva to $N > 4$ is, however, challenging. It would also be interesting to extend the studies presented in this paper to finite s -wave scattering lengths and to Bose droplets with an impurity.

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- [54] The Supplemental Material at [To Be Inset by the editor] contains tables for the energies for the models $2b\text{ZR}+3b\text{Rp}$ with $p = 4 - 8$, He-He(scale), and He-He(arctan).
- [55] In practice, the structural properties are obtained by calculating thermal averages at low temperature, where the excitations of the relative degrees of freedom are negligible. This implies that thermally averaged structural properties that are independent of the center of mass degrees of freedom coincide, to a very good approximation, with the corresponding quantum mechanical expectation values with respect to the ground state wave function.

Supplemental Material

Energy and structural properties of N -boson clusters attached to three-body Efimov states: Two-body zero-range interactions and the role of the three-body regulator

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The PIMC energies reported in Table II of the main text were obtained using the “fourth-order propagator” described in Ref. [1] using a fixed time step of $0.00045/E_3$. Table S1 summarizes the energies obtained by extrapolating the energies obtained using the second-order propagator for 3-4 different time steps to the zero time step limit. Comparison of Table II of the main text and Table S1 shows that the energies for the model 2bZR+3bRp with $p = 5 - 7$ obtained by the two different approaches agree within error bars (for $p = 4$ and 8, we did not perform calculations using the fourth-order propagator).

TABLE S1: PIMC energies for the model 2bZR+3bRp for $N = 5 - 15$. Columns 2-6 show the scaled energy $E_N/N/(E_3/3)$ for $p = 4-8$, respectively. The error bars (not explicitly reported) are around 6%.

N	2bZR+3bR4	2bZR+3bR5	2bZR+3bR6	2bZR+3bR7	2bZR+3bR8
5	5.58	6.36	6.67	6.70	6.63
6	8.22	8.90	9.53	10.2	10.4
7	8.96	11.1	12.1	12.3	13.4
8	10.4	12.9	14.8	15.6	16.2
9	11.6	14.8	16.8	18.1	18.7
10	12.7	16.5	17.9	20.0	21.2
11	13.1	18.0	20.5	22.0	23.2
12	13.5	18.7	22.0	23.8	25.3
13	13.5	20.0	23.5	25.7	27.6
14	14.3	20.9	24.8	27.6	29.1
15	14.6	21.5	25.9	28.9	30.5

Table S2 reports our DMC energies, obtained by extrapolating energies for 4-5 finite time steps to the zero time step limit, for the models He-He(scale) and He-He(arctan) [2].

TABLE S2: DMC energies for the Hamiltonian with two-body van der Waals interactions for $N = 4 - 15$. Columns 2-3 show the scaled energy $E_N/N/(E_3/3)$ for the models He-He(scale) and He-He(arctan), respectively. The error bars (not explicitly reported) are around 1%.

N	He-He(scale)	He-He(arctan)
4	3.952	3.936
5	7.761	7.737
6	11.81	11.78
7	15.86	15.80
8	19.76	19.67
9	23.50	23.38
10	27.06	26.87
11	30.40	30.11
12	33.60	33.26
13	36.60	36.18
14	39.45	38.81
15	42.16	41.66

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